puted stably with limited precision arithmetic. More complex models, long-ranged forces and other procedures for computation are being investigated.

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Perturbation Treatment of High-Energy-Electron Diffraction from Imperfect Crystals*

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A modified-Bloch-wave expansion is used to develop a theory of high-energy-electron diffraction from imperfect crystals. To compute these new Bloch waves one must solve a linear hyperbolic system in n unknowns. Scattering among the Bloch waves is controlled by the matrix elements of the perturbing potential, and various approximations to this scattering are discussed. The hyperbolic system is transformed to normal form; in making this transformation, the unknown functions become the plane-wave amplitudes of the Darwin representation. The normal form reveals the region of determinacy of the system: a cone generated by the diffracted beams. The contraction of this cone to a line (the column approximation) is discussed in terms of the Bloch-wave scattering.

I. INTRODUCTION

In the analysis of high-energy-electron diffraction from crystal defects, one never loses sight of the periodicity of the perfect crystal. This motivates one to begin with one of the well-understood representations for the perfect-crystal wave function, and then modify it in such a fashion as to render theoretical calculations and experimental analysis tractable.

The two common representations for the wave functions are the Bloch representation and the Darwin representation. In the Bloch representation, the wave function ψ is expressed as a linear combination of the eigenfunctions of the perfect-crystal Hamiltonian, which is always of the form $F_k(\vec{r})e^{i\vec{k}\cdot\vec{r}}$, where $F_k(\vec{r})$ is a periodic function of the crystal lattice. In the Darwin representation, one expands ψ as a summation of plane waves, with spatially varying amplitudes, traveling in the various diffraction directions as specified by Bragg's law.

Surprisingly, the modification of these representations to include nonperiodic distortions associated with crystal defects has been almost exclusively directed toward the Darwin representation.[1,2] In order to complement these approaches, we shall here begin with a modified Bloch representation in which the amplitudes to excite various Bloch states are changed from the constants θ^j of the perfect crystal to slowly varying functions of position $\theta^j(\vec{r})$ in the defect crystal. Wilkens[3] and later Howie and Basinski[2] have considered expansions with modified Bloch waves, but either initially (Howie and Basinski) or early in the derivation (Wilkens) they restrict the variation in $\theta^j(\vec{r})$ to z dependence, where z is a coordinate parallel to the zone axis of the diffracting planes. These treatments involve

either a column approximation or other restrictions (discussed in Sec. III E) that we wish to avoid here.

In agreement with other treatments, we shall take slowly varying to mean that $\nabla^2\theta^j(\vec{r})$ can be neglected in comparison with other terms. This approximation is made for mathematical expediency. However, unlike other derivations, we shall not initially assume that the perturbing portion of the Hamiltonian is slowly varying, or that the $\theta^j(\vec{r})$ are any more slowly varying than is consistent with the neglecting of the Laplacian.

We shall insert our modified Bloch expansion into the Schrödinger equation in which the Hamiltonian is written as the sum of the perfect-crystal Hamiltonian H_0 and a perturbing term H_1. We are assuming only elastic scattering so that the total energy of the electron is fixed by the energy of the electron beam incident on the specimen. We will be looking for solutions of the form $\psi = \sum_j \theta^j(\vec{r})B^j(\vec{r})$, where the Bloch functions $B^j(\vec{r})$ are eigenfunctions of H_0. Making use of the orthogonality of the Bloch states, we shall derive a system of partial differential equations for the $\theta^j(\vec{r})$.

The differential equations for $\theta^j(\vec{r})$ form a linear hyperbolic system of the form $\underline{L}\,\underline{\Theta} = \underline{Q}\,\underline{\Theta}$, where $\underline{\Theta}$ is a column vector containing the $\theta^j(\vec{r})$, $\underline{L}$ is a linear operator consisting of derivatives with matrix coefficients containing information from the perfect crystal, and $\underline{Q}$ is the inhomogeneous term that depends on the perturbation.

Next, we shall explore various scattering approximations that may be used to simplify the inhomogeneous term. Then, in order to simplify the derivative terms of $\underline{L}$, we shall transform the system to normal form. In normal form the derivatives become directional derivatives along various characteristic directions, and we will demonstrate that these characteristic directions correspond to diffracted beam directions. In two dimensions the region of determinacy for the solution of the system, generated by the characteristics, will be shown to be defined by the Takagi triangle.[1]

In making the transformation to normal form, the $\theta^j(\vec{r})$ are linearly transformed into new variables, termed characteristic variables. We shall identify these new unknowns as the plane-wave amplitudes of the Darwin representation, thus clearly demonstrating how one representation is naturally transformed into the other, an observation usually absent in previous discussions of the dynamical theory of high-energy-electron diffraction. Within each representation, we shall see the importance of the Fourier components of $H_1(\vec{r})$ in determining various scattering transitions.

Finally, we will demonstrate how the equations in either representation degenerate to a column approximation when only one derivative, the z derivative, is considered important. We will also discuss the restrictions placed upon the solutions by making this approximation.

In summary, we present here a new approach, through the Bloch-wave formalism, to the problem of the propagation of high-energy electrons in near-periodic structures. The rewards of this approach include (a) the concept of a local dispersion surface for Bloch-wave scattering, (b) a clear demonstration of the region of determinacy in crystal space for such scattering, (c) the identification of the plane-wave amplitudes of the Darwin representation with the characteristic variables of our differential system, and (d) a unification of existing theories[1-3] through the derivation and systematic examination of the very general differential equation that we abstract from the Schrödinger equation.

II. SYNOPSIS OF PERFECT-CRYSTAL EQUATIONS

A. Representations

When solving the perfect-crystal Schrödinger equation, $H_0\psi = E\psi$, one usually employs either the Bloch representation or the Darwin representation for the electron wave functions.[4]

For a crystal containing n beams (i.e., a transmitted beam and $n-1$ diffracted beams) the wave function in the Bloch representation is written

$$\psi = \sum_j \theta^j B^j(\vec{r}) \quad , \tag{1}$$

where j (and later i) $= 1, 2, \ldots, n$, because of Bloch-wave degeneracy, θ^j is a constant,

$$B^j(\vec{r}) = \sum_l C^j_{g(l)} e^{i[\vec{k}(j)+\vec{g}(l)]\cdot\vec{r}} \quad ,$$

$|\vec{k}(j)| = 2\pi/\lambda(j)$, $C^j_{g(l)}$ is the Bloch-wave amplitude coefficient, $\vec{g}(l)$ is a compressed notation for the reciprocal-lattice vector corresponding to the diffracting planes (hkl), and l (and later m and h) $= 1, 2, \ldots, n$. In this convention $\vec{g}(1)$ corresponds to the transmitted beam with $|\vec{g}(1)| = 0$. The term $\vec{g}(l)$, where $l > 1$, corresponds to a diffracted beam with $|\vec{g}(l)| = 2\pi/d(l)$, where $d(l)$ is the interplanar spacing of the diffracting planes represented by $\vec{g}(l)$.

For the Darwin representation, we have

$$\psi = \sum_l \varphi_{g(l)}(\vec{r}) D_l(\vec{r}) \quad , \tag{2}$$

where $\varphi_{g(l)}(\vec{r})$ are spatially varying amplitude coefficients, and

$$D_l(\vec{r}) = e^{i[\vec{k}+\vec{g}(l)]\cdot\vec{r}} \, .$$

Here we are denoting $D_l(\vec{r})$ as a plane wave in the $\vec{k}+\vec{g}(l)$ direction, where $\vec{k}$ is the vacuum wave vector corrected for index of refraction effects.

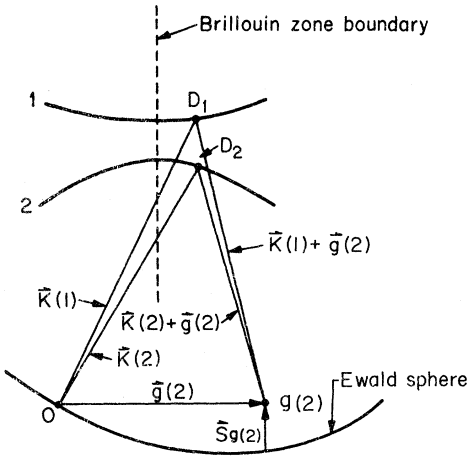

FIG. 1. Two-beam dispersion surface and associated Ewald sphere. This figure is not drawn to scale. The points D_1 and D_2 on branches 1 and 2, respectively, define the excited Bloch-wave vectors.

B. Solutions in Both Representations

When considering only perfect crystals, and neglecting absorption, the elements appearing in Eqs. (1) and (2) may be determined quite easily.

First, and this is necessary for either representation, one constructs a mean wave vector $\vec{k}$ which satisfies the two conditions (i) $|\vec{k}|^2+u_0=|\vec{\chi}|^2$ and (ii) $\vec{k}_t=\vec{\chi}_t$, where u_0 is the normalized Fourier component of the mean inner potential of the crystal and $\vec{\chi}$ is the wave vector of a monochromatic beam of electrons incident on the crystal specimen. Condition (i) expresses the conservation of energy for elastic Bragg scattering. Condition (ii) expresses the tangential continuity of the wave vectors, as dictated by the boundary conditions at the entrance surface of the crystal.

In order to determine the unknowns of the Bloch representation, one makes use of the Schrödinger equation in reciprocal space, which is an infinite number of simultaneous algebraic equations for the unknowns $C^j_{g(l)}$ of Eq. (1). Restricting the total number of beams that exist within the crystal to a finite number n, one obtains the perfect-crystal eigenvalue problem

$$\underline{A}\,\underline{C}^j-\gamma(j)\underline{C}^j=0 \quad , \tag{3}$$

where the $n\times n$ eigenvalue matrix $\underline{A}$ is constructed with the Fourier-potential coefficients and the Bragg deviation parameters $S_{g(l)}$, which describe the angular deviation of the incident beam from the classical Bragg angle for the reflections $\vec{g}(l)$. The elements of the $\underline{A}$ matrix are given by

$$[\underline{A}]_{lm}=\begin{cases} S_{g(l)} \ , & \text{for } l=m \\ u_{g(l-m)}/2k \ , & \text{for } l\neq m \ . \end{cases}$$

Here $u_{g(l-m)}$ is the Fourier coefficient of the lattice potential corresponding to the atomic planes with the reciprocal-lattice vector $\vec{g}(l-m)$, where $\vec{g}(l-m)=\vec{g}(l)-\vec{g}(m)$. Also, the reciprocal-lattice vector $\vec{g}(l-m)$ need not be an element of the initial set $\{\vec{g}(l)\,|\,l=1,2,\ldots,n\}$. The $\vec{g}(l)$ vectors are assumed to lie in an xy plane in reciprocal space so that solution of Eq. (3) yields the eigenvalues $\gamma(j)=k_z-k_z(j)$ and the eigenvectors $\underline{C}^j$, which are column vectors with elements $[\underline{C}^j]_l=C^j_{g(l)}$. The constants θ^j, which are the remaining unknowns that must be determined for the construction of the Bloch functions, are specified by the boundary conditions at the entrance surface of the crystal.

The plane-wave amplitudes $\varphi_{g(l)}(\vec{r})$ of the Darwin representation are only functions of z and may be determined by either a linear transformation $\underline{P}(z)$ from the Bloch representation, i.e.,

$$\underline{\Phi}(z)=\underline{P}(z)\underline{\Theta} \quad , \tag{4}$$

where $\underline{\Phi}(z)$ is a column vector with elements $[\underline{\Phi}(z)]_l=\varphi_{g(l)}(z)$ and $\underline{\Theta}$ is a column vector with elements $[\underline{\Theta}]_l=\theta^l$, or by the solution of the ordinary system

$$\frac{d}{dz}\underline{\Phi}=i\underline{A}\,\underline{\Phi} \quad , \tag{5}$$

where $\underline{A}$ is as defined above. Equation (5) has the formal solution

$$\underline{\Phi}(z)=e^{i\underline{A}z}\,\underline{\Phi}(0) \ .$$

The solution of the perfect-crystal eigenvalue problem may be displayed in reciprocal space as the dispersion-surface construction. Such a surface, with its associated Ewald-sphere construction, is shown for a two-beam case in Fig. 1. More generally, the excitation of n beams generates a dispersion surface of n branches (see Fig. 2).

III. IMPERFECT-CRYSTAL EQUATIONS

A. Derivation of Perturbation Equations

The imperfect-crystal Hamiltonian may be written H_0+H_1, where H_0 is the perfect-crystal Hamiltonian containing the kinetic and periodic potential energy operators and H_1 is an operator representing the deviation of the potential energy from that associated with perfect-crystal periodicity. We shall assume that only elastic scattering occurs, so that the total energy of the electrons inside the crystal is the same as that of the incident electron beam. The equation to be solved is

$$(H_0+H_1)\psi=E\psi \quad , \tag{6}$$

where we shall let ψ become the modified Bloch expansion

$$\psi=\textstyle\sum_j \theta^j(\vec{r})B^j(\vec{r}) \ . \tag{7}$$

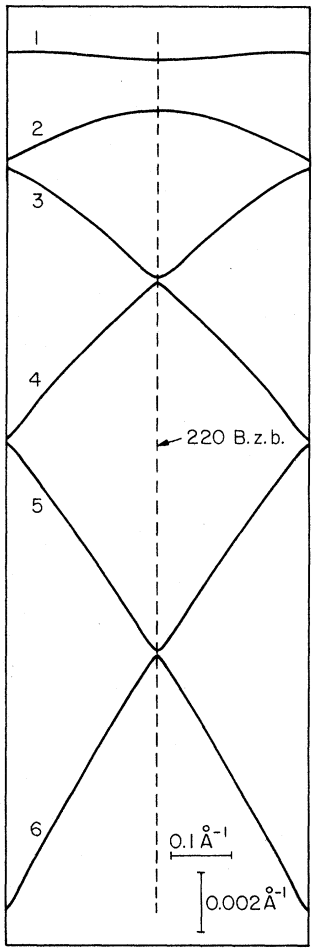

FIG. 2. Sample many-beam dispersion surface for a germanium crystal. The branches were calculated assuming six systematic reflections ($\bar{4}\bar{4}0$, ..., 660) are operating.

The summation in Eq. (7) extends over the n perfect-crystal Bloch functions $B^j(\vec{r})$. One may interpret Eq. (7) as revealing that (i) at a fixed point $\vec{r}$ within the crystal there is a distribution of the perfect-crystal Bloch functions $B^j(\vec{r})$ that differs from the distribution excited at the entrance surface, and this distribution is determined by the n numbers $\theta^j(\vec{r})$, or that (ii) within a region about the point $\vec{r}$ the behavior of the n functions $\theta^j(\vec{r})$ reveals the excitation of perturbed Bloch functions $\theta^j(\vec{r})B^j(\vec{r})$ which generally have wave vectors different from those of the perfect crystal. [We shall elaborate on interpretation (ii) in Sec. III F.]

Inserting ψ from Eq. (7) into Eq. (6), dotting $B^j(\vec{r})$ into both sides, and using the orthogonality relation

$$(B^i, B^j) \equiv \int_\tau \int B^{i*}(\vec{r})B^j(\vec{r})\,dx\,dy \cong \tau\delta_{ij} \ ,$$

where τ is the area of the intersection of the unit cell and the x-y plane, one obtains

$$k_z(i)\frac{\partial\theta^i}{\partial z} = \frac{i}{2\tau}\sum_j\left[(B^i, H_1\theta^jB^j) + 2\frac{\partial\theta^j}{\partial z}\left(B^i, \frac{\partial}{\partial x}B^j\right) + 2\frac{\partial\theta^j}{\partial y}\left(B^i, \frac{\partial}{\partial y}B^j\right)\right] . \quad (8)$$

In deriving Eq. (8) $\nabla^2\theta^j(\vec{r})$ has been neglected and the components of $\nabla\theta^j(\vec{r})$ have all been assumed to be constant within the region τ.

Now, it can be shown (see Appendix A) that the terms $(B^i, (\partial/\partial x)B^j)$ and $(B^i, (\partial/\partial y)B^j)$ appearing in Eq. (8) can be written

$$\left(B^i, \frac{\partial}{\partial x}B^j\right) \cong i\tau\left(k_x(j)\delta_{ij} + e^{ik_z(j-i)z}\sum_l C^j_{g(l)}C^{i*}_{g(l)}g_x(l)\right), \quad (9a)$$

$$\left(B^i, \frac{\partial}{\partial y}B^j\right) \cong i\tau\left(k_y(j)\delta_{ij} + e^{ik_z(j-i)z}\sum_l C^j_{g(l)}C^{i*}_{g(l)}g_y(l)\right), \quad (9b)$$

where $k_z(j-i) = k_z(j) - k_z(i)$ and $g_x(l)$ and $g_y(l)$ are the x and y components of the $\vec{g}(l)$ vectors. The exact equality in Eqs. (9a) and (9b) holds in the symmetrical Laue case.

B. Matrix Representation

In order to facilitate further manipulations with the perturbation equations, we will transform them to matrix form.

First, we will define the matrix $\underline{T}_x$ with elements

$$[\underline{T}_x]_{ij} = e^{ik_z(j-i)z}\sum_l C^j_{g(l)}C^{i*}_{g(l)}g_x(l)$$

and a similar expression for $\underline{T}_y$ with elements $[\underline{T}_y]_{ij}$ which are formed by replacing $g_x(l)$ with $g_y(l)$. Next, we define a column vector $\underline{H}\underline{\Theta}$ with elements

$$[\underline{H}\underline{\Theta}]_i = \sum_j (B^i, H_1\theta^jB^j) \ ,$$

and define a diagonal matrix $\underline{K}_z$ with elements

$$[\underline{K}_z]_{ij} = k_z(i)\delta_{ij} \ ,$$

and in a similar fashion as $\underline{K}_z$ we define the matrices $\underline{K}_x$ and $\underline{K}_y$.

Substituting these matrices into Eq. (8) and simplifying further by defining two new matrices

$$\underline{M}(z) \equiv \underline{K}_z^{-1}(\underline{K}_x + \underline{T}_x)$$

and

$$\underline{N}(z) \equiv \underline{K}_z^{-1}(\underline{K}_y + \underline{T}_y) \ ,$$

we obtain

$$\left(\frac{\partial}{\partial z} + \underline{M}(z)\frac{\partial}{\partial x} + \underline{N}(z)\frac{\partial}{\partial y}\right)\underline{\Theta}(\vec{r}) = \frac{i}{\tau}\underline{K}_z^{-1}\underline{H}\underline{\Theta}(\vec{r}) \ , \quad (10)$$

where $\underline{\Theta}(\vec{r})$ is a column vector with elements $[\underline{\Theta}]_i = \theta^i(\vec{r})$.

Equation (10) is a linear hyperbolic system for

the unknown function vector $\underline{\Theta}(\vec{r})$. This equation is linear because none of the derivative coefficients involves $\underline{\Theta}(\vec{r})$, and the inhomogeneous term involves $\underline{\Theta}(\vec{r})$ linearly. It is hyperbolic because all the eigenvalues of the matrices $\underline{M}$ and $\underline{N}$ are distinct (see Appendix B) and the system may thus be transformed into normal hyperbolic form.

C. Scattering Approximations

All of the effects of the perturbation are contained in the inhomogeneous term of Eq. (10). Each of the derivative (matrix) coefficients makes use of only information from the perfect crystal. It is also clear that as the crystal distortion vanishes (i.e., $H_1 \to 0$) the unique solution of the homogeneous problem is $\underline{\Theta}(\vec{r}) = \underline{\Theta}(0)$, where $\underline{\Theta}(0)$ is the column vector formed from the constants θ^j of the perfect crystal.

The inhomogeneous term may be left as it is, leaving what should really be termed a differentio-integral hyperbolic system, or two other possible approximations can be made, which we shall term the kinematical and Born cases. These three possibilities are summarized:

$$[\underline{H}\,\underline{\Theta}]_i = \sum_j \begin{cases} (B^i, H_1\theta^j B^j)\,, & \text{dynamical} \quad (11a) \\ (B^i, H_1 B^j)\theta^j(\vec{r})\,, & \text{kinematical} \quad (11b) \\ (B^i, H_1 B^j)\theta^j(0)\,, & \text{Born}\,. \quad (11c) \end{cases}$$

Let us recall the restrictions that we have placed upon the $\theta^j(\vec{r})$ functions. They are slowly varying in the sense that $\nabla^2\theta^j(\vec{r})$ can be neglected. Now consistent with this restriction is our assumption that the gradient of $\theta^j(\vec{r})$ remains constant enough throughout the region of integration τ, so that it may be removed from the integrals. By making these assumptions we are able to (i) avoid the complexities of coupled second-order equations and (ii) convert terms such as $(B^i, (\partial\theta^j/\partial z)B^j)$ to $(\partial\theta^j/\partial z)(B^i, B^j)$, thereby allowing us to uncouple some otherwise coupled terms through the use of the orthogonality of the Bloch states. However, at this level of approximation we cannot remove $\theta^j(\vec{r})$ from these integrals, and so we see it in the dynamical term of Eq. (11a).

There may well be cases when we need not be so rigorously restrictive, and so we may take advantage of these cases to modify our inhomogeneous term, as shown in Eqs. (11b) and (11c). One can easily justify these approximations with arguments of mathematical expediency, but what can we say of their physical justification?

Interpreting $\theta^j(\vec{r})B^j(\vec{r})$ as a perturbed Bloch wave, we see that common to all three scattering approximations is the usual quantum-mechanical result that the rate of change of the $\theta^j(\vec{r})$ functions is controlled by matrix elements of the form $(B^i, H_1 B^j)$, where $B^i(\vec{r})$ and $B^j(\vec{r})$ represent either perfect or perturbed Bloch functions. In other words, the amplitude to excite a transition from the state B^i to the state B^j, summed over all possible B^j, determines the rate of change of the amplitude for B^i to exist.

The kinematical approximation restricts the Bloch functions that determine the transition amplitudes to perfect-crystal Bloch functions. This restriction on what transitions can contribute to the matrix elements is reflected in greater restrictions on the slowly varying nature of the $\theta^j(\vec{r})$ function. Now, not only must $\nabla\theta^j(\vec{r})$ be constant within τ, but also the $\theta^j(\vec{r})$, enabling us to remove them from the scattering integral, as shown in Eq. (11b). Should the perturbation be such that the dynamical scattering of Eq. (11a) is required, the kinematical approximation may be the first step in an iterative integration approach to the solution of the system of Eq. (10).

Even weaker scattering can be handled by the Born approximation to the perturbation. A prerequisite to the application of this approximation is that the perturbation be sufficiently localized so that only slight scattering occurs (e.g., a condition one would anticipate for point defects). Wilkens[3] has used this scattering approximation coupled with the column approximation to predict the transmission-electron-microscope-image widths of small spherical inclusions.

Although throughout the remainder of this paper we shall make use of the kinematical approximation, it should be noted that all the results obtained are valid for the dynamical case if one remembers to interpret the perturbation terms $\underline{H}$ and later $\underline{\mathcal{K}}$ as integral operators.

As we have pointed out, one may interpret the waves $\theta^j(\vec{r})B^j(\vec{r})$ as perturbed or distorted Bloch waves, that is to say, there exist Bloch waves within the imperfect crystal whose wave vectors differ from those of the perfect crystal. These new wave vectors can be defined only locally, of course, since their existence is made possible by the local distortion, and in general we would not expect such locally excited waves to be able to propagate into new regions without subsequent modulation. By "locally about a point" we mean a region whose extent in the x-y plane is an area identical to the region of integration used previously and which is of a differential thickness dz. The region must enclose the point, but other than this restriction the point may be anywhere within the area. By defining "locally" in this way, we assure ourselves of being able to discuss the behavior of solutions of the differential equation about a point, and simultaneously partition up our crystal space into distinct cells that completely fill that space.

Within this region we expect to have a local reciprocal lattice and a local dispersion surface con-

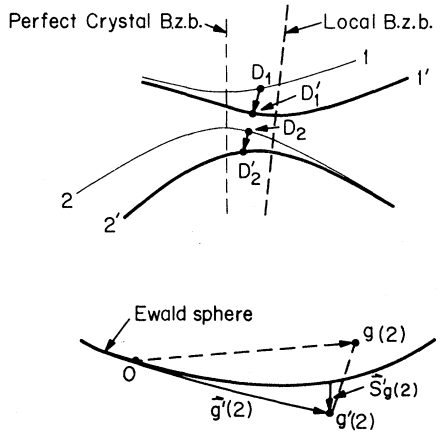

FIG. 3. Local two-beam dispersion surface (heavy lines) with the perfect-crystal dispersion surface (light lines) shown for comparison. This drawing is not to scale and the primes refer to the local dispersion surface and reciprocal-lattice vector. In this example the deviations from the perfect-crystal conditions are manifest by a shift in the reciprocal-lattice vector $\vec{g}(2)$ to $\vec{g}'(2)$ and the excitations of the Bloch waves defined by the points D_1' and D_2'.

sistent with the departure of the potential energy function from its perfect-crystal periodicity. This new dispersion surface is shown superimposed with the perfect-crystal surface for the two-beam case in Fig. 3. In order to conserve energy we require that the local wave vectors lie on this surface. Also, if the region of distortion has a well-defined boundary separating it from the perfect crystal, one may further require the tangential continuity of the wave vectors across such a boundary. We see from Fig. 3 that the effect of the transition to the new dispersion surface is to alter the distance of the excited wave vectors from the local Brillouin-zone boundary (Bzb). In other words, the distortion acts to either bring the waves closer to or farther from the exact Bragg condition. One sees this both on the dispersion surface and at the reciprocal-lattice points as their deviation parameters $S_{g(l)}$ vary with depth. The reorientation of the wave vectors with respect to the new Bzb is primarily due to the movement of the reciprocal-lattice vectors; in Fig. 3 we see how the movement of the reciprocal point $g(2)$ across the Ewald sphere to $g'(2)$ has taken two wave vectors originally to the right of the perfect crystal Bzb and transported them to the left of the local Bzb. From this we see how strong beams (e.g., at the exact Bragg condition) must move away from this condition in the presence of any distortion that alters the reciprocal lattice and suffer a corresponding loss in intensity. This is not to imply that an arbitrary perturbation must distort the reciprocal lattice. For example, we can be assured that strain fields will indeed distort the lattice, while a simple structure-factor change might not cause appreciable distortion, acting only to bring the dispersion-surface branches closer together (or push them apart) while preserving the Bzb.

It is usual to speak of two types of transitions which occur simultaneously on the dispersion surface: intraband and interband transitions. We have been considering the intraband process; this involves transitions occurring as the result of a small momentum transfer from the perfect-crystal branch to its associated local branch.

By interband transitions we merely mean that we acknowledge the inherent coupling of any particular $\theta^j(\vec{r})$ to all the other $\theta^i(\vec{r})$ through the differential equation. Some of these functions grow (in the sense of suitable norm) at the expense of others. Physically, electrons are being continually redistributed (i.e., scattered) from states represented by one branch of the dispersion surface to another. In particular, the intraband transition is the coupling of $\theta^j(\vec{r})$ to itself through the differential equation; hence, one can always separate the inhomogeneous term of Eq. (10) into the sum of an intraband coupling and interband couplings. Then, if one can eliminate the intraband term through some transformation (this is explicity done for a special case in Sec. III E), the intraband process is then completely determined and one can exhibit the local dispersion surface.

D. Transformation to Normal Form

If, for simplicity, we restrict ourselves to two independent variables, then Eq. (10) may be rewritten

$$\left(\frac{\partial}{\partial z}+\underline{M}(z)\,\frac{\partial}{\partial x}\right)\underline{\Theta}(\vec{r})=\frac{i}{2\tau}\,\underline{K}_g^{-1}\underline{H}\,\underline{\Theta}(\vec{r})\ . \tag{12}$$

We want to transform Eq. (12) to the form

$$\underline{D}\,\underline{\Phi}=\underline{B}\,\underline{\Phi}\ , \tag{13}$$

where $\underline{D}$ is a diagonal matrix of directional derivative operators

$$\frac{\partial}{\partial n^l}\equiv\frac{\partial}{\partial z}+\alpha^l\,\frac{\partial}{\partial x}$$

which differentiates the characteristic variables $\varphi_{g(l)}$ along n different characteristic directions and $\underline{B}$ is a matrix independent of the $\varphi_{g(l)}$ and is obtained linearly from the matrices of Eq. (12).

To make such a transformation it is necessary only to solve the eigenvalue problem for the matrix $\underline{M}$. Suppose we have found the n eigenvalues α^l and the n eigenvectors $\vec{\mathrm{P}}^l$. Then form the eigenvector matrix P with elements

$[\underline{P}]_{lm}=\vec{\mathrm{P}}^l$ for the row l. Next we make the trans-

formation to the characteristic variables $\varphi_{g(l)}$ through $\underline{\Phi} = \underline{P}\,\underline{\Theta}$. Putting $\underline{\Theta} = \underline{P}^{-1}\underline{\Phi}$ into Eq. (12) we obtain

$$\left[\underline{P}^{-1}\frac{\partial}{\partial z} + \left(\frac{\partial}{\partial z}\underline{P}^{-1}\right) + \underline{M}\left(\frac{\partial}{\partial x}\underline{P}^{-1}\right) + \underline{M}\underline{P}^{-1}\frac{\partial}{\partial x}\right]\underline{\Phi} = \frac{i}{2\tau}\underline{K}_z^{-1}\underline{H}\underline{P}^{-1}\underline{\Phi} \ .$$

Now, premultiplying by $\underline{P}$, we obtain

$$\left(\frac{\partial}{\partial z} + \underline{P}\underline{M}\underline{P}^{-1}\frac{\partial}{\partial x}\right)\underline{\Phi} = \left[\frac{i}{2\tau}\underline{P}\underline{K}_z^{-1}\underline{H}\underline{P}^{-1} - \underline{P}\left(\frac{\partial}{\partial z}\underline{P}^{-1}\right) - \underline{P}\underline{M}\left(\frac{\partial}{\partial x}\underline{P}^{-1}\right)\right]\underline{\Phi} \ .$$

But $\underline{P}\underline{M}\underline{P}^{-1}$ is a diagonal matrix with elements

$$[\underline{P}\underline{M}\underline{P}^{-1}]_{lm} = \alpha^l \delta_{lm} \ ,$$

so we have

$$\underline{D}\,\underline{\Phi} = \underline{B}\,\underline{\Phi} \ ,$$

where

$$\underline{B} = \left[\frac{i}{2\tau}\underline{P}\underline{K}_z^{-1}\underline{H}\underline{P}^{-1} - \underline{P}\left(\frac{\partial}{\partial z}\underline{P}^{-1}\right) - \underline{P}\underline{M}\left(\frac{\partial}{\partial x}\underline{P}^{-1}\right)\right] .$$

In principle, this can always be done, and Eq. (13) is the equation to integrate. However, the mathematics obscures the physics unless one makes the approximations that $\underline{K}_z \cong k_z \underline{I}$ and $\underline{K}_x \cong k_x \underline{I}$, where k_z is a mean $k_z(l)$, which we shall freely set equal to $|\vec{k}|$, k_x is a mean $k_x(l)$ (this last distinction need not be made in the symmetrical Laue case), and $\underline{I}$ is the identity matrix. We then can write

$$\underline{M} = \underline{K}_z^{-1}(k_x \underline{I} + \underline{T}_x)$$

and show (see Appendix B) that the eigenvalues of $\underline{M}$ are

$$\alpha^l = \frac{k_x}{k_z}, \ \frac{k_x + |\vec{g}(2)|}{k_z}, \ \cdots, \ \frac{k_x + |\vec{g}(n)|}{k_z} \ .$$

The eigenvalues α^l determine the characteristic directions through the ordinary differential equations (which are trivial to integrate in this case) $dx^l/dz = \alpha^l$. In general, these differential equations define curves $x^l(z)$ in the x-z plane that determine the direction of propagation of information. In this case, since the α^l are constant, the curves are merely straight lines with slopes α^l.

Under this same approximation for $\underline{M}$ one finds that the eigenvector matrix $\underline{P}$ is identical to the transformation matrix from the Bloch to the Darwin representation defined by Eq. (4). Thus, the characteristic variable column vector $\underline{\Phi}$ is identified as the vector containing the plane-wave amplitudes of the Darwin representation.

So we learn about the various terms of the $\underline{B}$ matrix of Eq. (13):

$$\frac{\partial}{\partial x}\underline{P}^{-1} = 0 \ , \quad \underline{P}\left(\frac{\partial}{\partial z}\underline{P}^{-1}\right) = -i\underline{A} \ .$$

The elements of the perturbation term transform according to

$$[\underline{P}\underline{H}\underline{P}^{-1}]_{lm} = (G_l, H_1 G_m) \ ,$$

where

$$G_l = e^{i\vec{g}(l)\cdot\vec{r}} \ .$$

Defining the matrix $\underline{\mathcal{K}}$ with elements

$$[\underline{\mathcal{K}}]_{lm} = (G_l, H_1 G_m) \ ,$$

we see that the perturbation transforms simply as $\underline{P}\underline{H}\underline{P}^{-1} = \underline{\mathcal{K}}$ and Eq. (13) becomes the system

$$\underline{D}\,\underline{\Phi} = i\left(\underline{A} + \frac{1}{2k\tau}\underline{\mathcal{K}}\right)\underline{\Phi} \ . \qquad (14)$$

This is the perturbation modification of Eq. (5). Once again we see how the various matrix elements of the relevant transitions (in this case $G_l \rightarrow G_m$) determine the rate of change of the amplitude to find the electrons in a particular state. All that has really occurred is that an equivalence transformation has taken us from one set of basis vectors to another.

Referring to Fig. 4, we see that from any point P at the exit surface of a thin crystal specimen, one can draw the n characteristics determined by $dx^l/dz = \alpha^l$ where, for simplicity, we have taken $l = 1, 2$. We of course generate a triangle, and the family of lines parallel to the sides of this triangle generate a mesh within it. Given the initial values $\underline{\Phi}(0)$ at the entrance surface of the crystal, and a sufficiently smooth $\underline{\mathcal{K}}$ within PAB, the solution at P can be constructed by iterated integration of Eq. (14) along the n characteristics

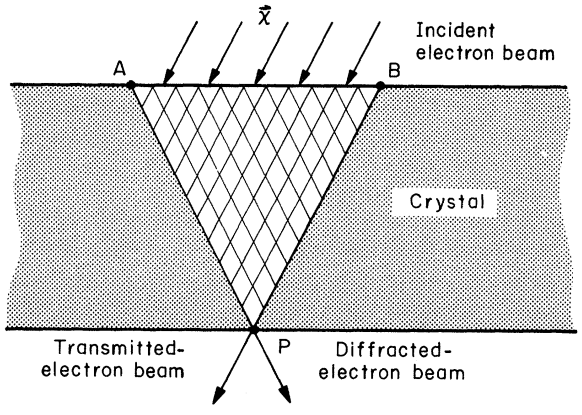

FIG. 4. Two-beam region of determinacy. The triangle PAB and its associated mesh are generated by the characteristics of the system and define the region of determinacy for the point P. The slopes of the sides of the triangle are given by the eigenvalues of the $\underline{M}$ matrix.

beginning with any convenient initial $\underline{\Phi}$ that satisfies the boundary conditions. Although we shall not present this procedure here, we note that it offers a demonstration of the existence of a solution $\underline{\Phi}(\vec{r})$, and a region of determinacy of the equation. This region, first described by Takagi[1] for a similar hyperbolic system, is bounded by the outermost characteristics defined by $\alpha^1 = \min[\alpha^l]$ and $\alpha^n = \max[\alpha^l]$. As Takagi has pointed out, these characteristics provide a theoretical basis for the column approximation (e.g., in Fig. 4, the distance A to B is about 20 Å for a crystal 1000 Å thick). In three dimensions the region of determinacy becomes a cone bounded by n triangular sides.

The advantage of writing the Hamiltonian as $H_0 + H_1$ is that not only strain contrast, but structure-factor contrast, can be included at any point. However, if we limit the discussion to slowly varying strain fields, and employ the deformable-ion approximation, we have

$$H_1(\vec{r}) = \sum_l u_{g(l)} e^{i\vec{g}(l)\cdot\vec{r}} (e^{-i\vec{g}(l)\cdot\vec{R}(\vec{r})} - 1) \ ,$$

where $\vec{R}(\vec{r})$ is a vector function describing the atomic displacement at $\vec{r}$. Then, with the slowly varying approximation

$$\begin{aligned}(G_l, H_1 G_m) &= \sum_h u_{g(h)} [G_l, (e^{-i\vec{g}(h)\cdot\vec{R}(\vec{r})} - 1) G_{h+m}] \\ &\cong \sum_h u_{g(h)} (e^{-i\vec{g}(h)\cdot\vec{R}(\vec{r})} - 1)(G_l, G_{h+m}) \\ &= u_{g(l-m)} (e^{-i\vec{g}(l-m)\cdot\vec{R}(\vec{r})} - 1) \ ,\end{aligned}$$

Eq. (14) becomes

$$\underline{D}\,\underline{\Phi} = i\underline{A}(\vec{r})\underline{\Phi} \ ,$$

where

$$[\underline{A}(\vec{r})]_{lm} = \begin{cases} S_{g(l)} \ , & \text{for } l = m \\ \dfrac{u_{g(l-m)}}{2k} \ e^{-i\vec{g}(l-m)\cdot\vec{R}(\vec{r})} \ , & \text{for } l \neq m. \end{cases}$$

Making the phase transformation

$$\varphi'_{g(l)}(\vec{r}) = \varphi_{g(l)}(\vec{r}) e^{i\vec{g}(l)\cdot\vec{R}(\vec{r})} \ ,$$

one obtains

$$\underline{D}\,\underline{\Phi}' = i\underline{A}'(\vec{r})\underline{\Phi}' \ , \tag{15}$$

where

$$[\underline{A}'(\vec{r})]_{lm} = \begin{cases} S_{g(l)} + \dfrac{\partial}{\partial n^l} [\vec{g}(l)\cdot\vec{R}(\vec{r})] \ , & \text{for } l = m \\ \dfrac{u_{g(l-m)}}{2k} \ , & \text{for } l \neq m. \end{cases}$$

Using a completely different approach, Takagi[1] has also obtained Eq. (15). His derivation begins with the Darwin representation and, with less generality than we make use of here, includes only the slowly varying strain field as a possible perturbation. Whatever the approach, one sees in Eq. (15) how this type of perturbation determines contrast through a local distortion of the reciprocal lattice, and consequent variation in the Bragg deviation parameters.

E. Column Approximation

Let us return to Eq. (10) and neglect the terms involving x and y derivatives, letting $\underline{\Theta}(\vec{r}) = \underline{\Theta}(z)$. This is the column approximation, motivated by the fact that the matrix coefficients $\underline{K}_x$, $\underline{K}_y$, $\underline{T}_x$, and $\underline{T}_y$ are all composed of elements whose magnitude is on the order of 1/50 of the elements of $\underline{K}_z$. Equation (10) then becomes

$$\underline{K}_z \frac{d}{dz} \underline{\Theta}(z) = \frac{i}{\tau} \underline{H}\,\underline{\Theta}(z) \ , \tag{16}$$

where now

$$[\underline{H}\,\underline{\Theta}]_i = \sum_j (B^i, H_1 B^j) \theta^j(z) \ .$$

As has been mentioned, Howie and Basinski[2] have also considered an expansion with modified Bloch waves, but they begin their study with only z dependence and so obtain the rather limited behavior of Eq. (16). Actually, they attempt to avoid the column approximation by allowing the summation over j to include other possible perfect-crystal Bloch waves, which seems rather artificial in that we do not really know what waves are propagating until we integrate the more complete equation (10).

However, with the restrictions here, Eq. (16) offers a column approximation in that the wave function at a depth z is uniquely determined by integration along a line from the entrance surface.

The application of the column approximation to analyze high-resolution transmission-electron-microscope images of crystal defects has proven to be quite dangerous. For instance, recent calculations[5,6] have shown that the column approximation breaks down when the principle contrast mechanism involves transitions from the higher (flatter) dispersion-surface branches to the lower kinetic-energy (more sharply peaked) branches. The group velocity of the Bloch waves excited on the lower branches, which is normal to the surface, tends to depart from the z direction, destroying the column approximation. Allowing the reverse transitions to predominate, one finds the column approximation valid again.

Writing out Eq. (16) explicitly, we have

$$\begin{aligned} k_g(i) \frac{d\theta^i}{dz} &= \frac{i}{2\tau} \sum_j \theta^j(z) \sum_{l,m} C^j_{g(l)} C^{i*}_{g(m)} e^{i k_g (j-i) z} \\ &\quad \times \int_\tau \int H_1 e^{i\vec{g}(l-m)\cdot\vec{r}} \, dx \, dy \\ &= \frac{i}{2\tau} \sum_{j,l,m} \theta^j(z) C^j_{g(l)} C^{i*}_{g(m)} e^{i k_g (j-i) z} (G_m, H_1 G_l) \ . \end{aligned}$$

So we have, making the Born approximation and after integrating both sides,

$$\theta^i(z)=\theta^i(0)+\frac{i}{2\tau}\sum_{j,l,m}\theta^j(0)C^j_{g(l)}C^{i*}_{g(m)}\int_0^z (G_m,H_1G_l)\times e^{ik_z(j-i)z'}\,dz' \ .$$

Here we see how transitions are controlled by an integral that picks out the Fourier components of (G_m, H_1G_l), the matrix elements of H_1, with respect to a wave-vector change in the z direction of $k_z(j-i)$. The $k_z(j-i)$ are approximately the separations of the various perfect-crystal dispersion-surface branches along the line of excitation.

Similarly, the column approximation to Eq. (14) is

$$\frac{d}{dz}\,\underline{\Phi}=i\left(\underline{A}+\frac{1}{2k\tau}\,\underline{\mathcal{K}}\right)\underline{\Phi} \ .$$

For the cases of slowly varying strains one can simplify this to

$$\frac{d}{dz}\,\underline{\tilde{\Phi}}=i\underline{A}'\,\underline{\tilde{\Phi}} \ , \tag{17}$$

where

$$[\underline{A}'(\vec{r})]_{lm}=\begin{cases} S_{g(l)}+\dfrac{d}{dz}\,[\vec{g}(l)\cdot\vec{R}(\vec{r})] \ , & \text{for } l=m \\ \dfrac{u_{g(l-m)}}{2k} \ , & \text{for } l\neq m \ . \end{cases}$$

Equation (17) is probably the most straightforward of the column approximation theories in terms of computational ease, since all that must be done is to locally vary the diagonal elements of the $\underline{A}'$ matrix as one numerically integrates along the z direction.

F. Separation of Intraband and Interband Transitions

The mathematics involved in extracting intraband and interband transitions from the differential equations may be best exemplified by the column approximation equations in the Bloch representation for slowly varying strains. We may easily obtain these equations by substituting $\underline{\Phi}=\underline{P}\,\underline{\Theta}$ into Eq. (17). After a few algebraic manipulations, one obtains the following system for the $\underline{\Theta}$ vectors:

$$\frac{d}{dz}\,\underline{\Theta}=i\,\underline{\Gamma}^*\underline{C}^{-1}\underline{E}\,\underline{C}\,\underline{\Gamma}\,\underline{\Theta} \ , \tag{18}$$

where $\underline{\Gamma}$ is a diagonal matrix with elements

$$[\underline{\Gamma}]_{ij}=e^{i\gamma(i)z}\delta_{ij} \ ,$$

$\underline{E}$ is a diagonal matrix with elements

$$[\underline{E}]_{lm}=\frac{d}{dz}\,[\vec{g}(l)\cdot\vec{R}(\vec{r})]\delta_{lm} \ ,$$

and $\underline{C}$ is the usual eigenvector matrix.

The matrix product on the right-hand side of Eq. (18) is not as formidable as it looks, since three of the matrices are diagonal. In component form this equation becomes

$$\frac{d}{dz}\,\theta^i=i\sum_{l,j}\frac{d}{dz}\,[\vec{g}(l)\cdot\vec{R}(\vec{r})]C^j_{g(l)}C^{i*}_{g(l)}e^{i\gamma(j-i)z}\,\theta^j \ , \tag{19}$$

where $\gamma(j-i)=\gamma(j)-\gamma(i)$.

In Eq. (19) all of the terms of the j summation, except the ith term, represent interband transitions, and the ith term represents intraband transitions from the surface i. Consequently, we may write the right-hand side of Eq. (19) as the sum of the intraband and interband scattering terms. Doing this we obtain

$$\frac{d}{dz}\,\theta^i=i\sum_l\left(\sum_{j\neq i}\frac{d}{dz}\,[\vec{g}(l)\cdot\vec{R}]C^j_{g(l)}C^{i*}_{g(l)}e^{i\gamma(j-i)z}\theta^j+\frac{d}{dz}\,[\vec{g}(l)\cdot\vec{R}]\,|C^i_{g(l)}|^2\theta^i\right) \ . \tag{20}$$

Now, the point of making this separation is to allow us to completely eliminate the intraband term through the phase transformation

$$\theta^i=\theta'^i e^{i\sigma(i)} \ , \tag{21}$$

where

$$\sigma(i)=\textstyle\sum_l\ |C^i_{g(l)}|^2[\vec{g}(l)\cdot\vec{R}(\vec{r})] \ .$$

Performing the transformation indicated in Eq. (21) on Eq. (20) we obtain

$$\frac{d}{dz}\,\theta'^i=i\sum_l\sum_{j\neq i}\frac{d}{dz}\,[\vec{g}(l)\cdot\vec{R}(\vec{r})]\times C^j_{g(l)}C^{i*}_{g(l)}e^{i[\gamma(j-i)z+\sigma(j-i)]}\theta'^j \ . \tag{22}$$

This differential system contains only interband terms. We see that the result of the intraband scattering is to effectively change the wave vector of the ith Bloch wave from $k_z(i)$ to $k_z(i')$, where $k_z(i')=k_z(i)+\sigma(i)/z$.

Thus, the local dispersion-surface branches, upon which the interband process will redistribute the Bloch amplitudes, can be obtained from the perfect-crystal branches by a translation in the z direction of

$$k_z(i'-i)=(1/z)\textstyle\sum_l\ |C^i_{g(l)}|^2[\vec{g}(l)\cdot\vec{R}(\vec{r})] \ .$$

IV. SUMMARY

In this paper, within the confines of our slowly varying assumption, we have presented a general treatment of high-energy-electron diffraction from imperfect crystals. Making use of a modified Bloch expansion, we have derived a first-order hyperbolic system for the spatially varying Bloch-wave excitation amplitudes and have demonstrated that the normal form of this system, under suitable

approximations, is merely a Darwin-representation expansion of the wave function. The region of determinacy of the system, essential to considerations of the applicability of the column approximation, has been shown to be generated by the solutions of a simple eigenvalue problem.

Most importantly, we have attempted to demonstrate the interdependence of the rather general equations derived here, and a multitude of rather specialized equations presented in the literature. Authors have brought forth Darwin expansions, Bloch expansions with z dependence, modified Bloch expansions with z dependence, and assorted column approximation equations, all seemingly without connection to one another. We have here shown how we are really only dealing with a single hyperbolic system and we may easily obtain any other particular system by merely making some convenient choice of representation, assumptions about the distortion, use of the entire region of determinacy, and scattering approximation.

We are currently working on the development of reliable guidelines that connect a particular type of imperfect crystal with the least complex combination of the above four choices that will still predict the wave function accurately.

APPENDIX A

The integral $(B^i, (\partial/\partial x)B^j)$ which appears in Eq. (8) is written in complete form as

$$\begin{aligned}\left(B^i, \frac{\partial}{\partial x} B^j\right) &\equiv \int_\tau \int B^{i*}(\vec{r}) \frac{\partial}{\partial x} B^j(\vec{r})\, dx\, dy \\ &= \sum_{l,m} \int_\tau \int C^j_{g(l)} C^{i*}_{g(m)} e^{-i[\vec{k}(i)+\vec{g}(m)]\cdot\vec{r}} \\ &\qquad \times \frac{\partial}{\partial x} e^{i[\vec{k}(j)+\vec{g}(l)]\cdot\vec{r}}\, dx\, dy \\ &= \sum_{l,m} i C^j_{g(l)} C^{i*}_{g(m)} [k_x(j) + g_x(l)] \\ &\qquad \times \int_\tau \int e^{i[\vec{k}(j-i)+\vec{g}(l-m)]\cdot\vec{r}}\, dx\, dy \ . \end{aligned} \tag{A1}$$

In Eq. (A1) we will neglect the terms $k_x(j-i)$ in comparison with the length of a $\vec{g}(l)$ vector. [This approximation is good to about one part in 500 for lower order $\vec{g}(l)$.] So we may write

$$\begin{aligned}\left(B^i, \frac{\partial}{\partial x} B^j\right) &\cong \sum_{l,m} i C^j_{g(l)} C^{i*}_{g(m)} [k_x(j) + g_x(l)]\, e^{ik_z(j-i)z} \\ &\qquad \times \int_\tau \int e^{i\vec{g}(l-m)\cdot\vec{r}}\, dx\, dy \\ &\cong i\tau \sum_l C^j_{g(l)} C^{i*}_{g(m)} [k_x(j) + g_x(l)]\, e^{ik_z(j-i)z} \\ &\cong i\tau [k_x(j)\delta_{ij} + e^{ik_z(j-i)z} \sum_l C^j_{g(l)} C^{i*}_{g(l)} g_x(l)]. \end{aligned} \tag{A2}$$

In a similar fashion as Eq. (A2), $(B^i, (\partial/\partial y)B^j)$, appearing in Eq. (8), becomes

$$\left(B^i, \frac{\partial}{\partial y} B^j\right) \cong i\tau \left(k_y(j)\delta_{ij} + e^{ik_z(j-i)z} \sum_l C^j_{g(l)} C^{i*}_{g(l)} g_y(l)\right). \tag{A3}$$

APPENDIX B

In order to determine the eigenvalues of

$$\underline{M} = \frac{1}{k_z} (k_x \underline{I} + \underline{T}_x) \ , \tag{B1}$$

we first define the diagonal matrix $\underline{\Omega}$ with elements

$$[\underline{\Omega}]_{ij} = e^{ik_z(i)z}\delta_{ij}$$

and the diagonal matrix $\underline{\Upsilon}$ with elements

$$[\underline{\Upsilon}]_{lm} = g(l)\delta_{lm} \ ,$$

so that $\underline{T}_x$ can be written

$$\underline{T}_x = \underline{\Omega}^* \underline{C}^* \underline{\Upsilon} \tilde{\underline{C}} \underline{\Omega} \ .$$

The eigenvalues of the $\underline{M}$ matrix will be unchanged if we transpose it so

$$\begin{aligned}\tilde{\underline{M}} &= \frac{1}{k_z} (k_x \underline{I} + \tilde{\underline{T}}_x) \\ &= \frac{1}{k_z} (k_x \underline{I} + \underline{\Omega}\underline{C}\underline{\Upsilon}\tilde{\underline{C}}^*\underline{\Omega}^*) \ . \end{aligned} \tag{B2}$$

The equation we must solve in order to determine the eigenvalues of equation (B2) is

$$\begin{aligned} &\| \tilde{\underline{M}} - \alpha \underline{I} \| = 0 \ , \\ &\left\| \left(\frac{k_x}{k_z} - \alpha\right) \underline{I} + \frac{1}{k_z} (\underline{\Omega}\underline{C}\underline{\Upsilon}\tilde{\underline{C}}^*\underline{\Omega}^*) \right\| = 0 \ . \end{aligned} \tag{B3}$$

Since $\underline{C}$ is unitary, $\tilde{\underline{C}}^* = \underline{C}^{-1}$, and we may write

$$\begin{aligned}\left(\frac{k_x}{k_z} - \alpha\right) \underline{I} &= \left(\frac{k_x}{k_z} - \alpha\right) \underline{\Omega}\underline{C}\underline{C}^{-1}\underline{\Omega}^* \\ &= \underline{\Omega}\underline{C} \left(\frac{k_x}{k_z} - \alpha\right) \underline{C}^{-1}\underline{\Omega}^* \ . \end{aligned} \tag{B4}$$

Substituting Eq. (B4) into Eq. (B3) we may write

$$\left\| \underline{\Omega}\underline{C} \left[\left(\frac{k_x}{k_z} - \alpha\right) \underline{I} + \frac{\underline{\Upsilon}}{k_z} \right] \underline{C}^{-1}\underline{\Omega}^* \right\| = 0 \ . \tag{B5}$$

Now, recalling that $\| \underline{A}\,\underline{B}\,\underline{C} \| = \| \underline{A} \| \cdot \| \underline{B} \| \cdot \| \underline{C} \|$, we may write for Eq. (B5)

$$\left\| \frac{1}{k_z} (k_x \underline{I} + \underline{\Upsilon}) - \alpha \underline{I} \right\| = 0 \ .$$

This implies that

$$\begin{aligned}\alpha^l &= \frac{1}{k_z} \{k_x + [\underline{\Upsilon}]_{ll}\} \\ &= \frac{1}{k_z} [k_x + |\vec{g}(l)|] \ . \end{aligned} \tag{B6}$$

Thus, the eigenvalues of the matrix $\underline{M}$ are given by Eq. (B6).

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Polarization Dependence of Shear-Wave Attenuation by Open-Orbit Electrons in Cu†

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The strength of measured resonant-attenuation peaks for ultrasonic shear waves caused by open-orbit electrons in Cu is shown to be related to the component of electron motion in the direction of sound polarization. The direction of the applied magnetic field is irrelevant except in determining the orbit geometry. The open orbit in Cu for $\vec{B} \parallel [101]$ has a much larger component of motion along $\vec{B}$ than perpendicular to it, so that interpretations of data based on motion in the plane perpendicular to $\vec{B}$ fail.

I. INTRODUCTION

It is usually stated[1] that magnetoacoustic resonances with shear waves are most pronounced when the external magnetic field $\vec{B}$ is perpendicular to the ultrasonic polarization vector $\vec{\epsilon}$. We report here a situation for which the open-orbit resonance is almost nonexistent for $\vec{B} \perp \vec{\epsilon}$. This observation not only sheds further light on the interaction responsible for the resonance, but it also illustrates the fallacy of ignoring electron motion along $\vec{B}$ in analyzing transport phenomena.

The open orbit which shows these anomalous effects arises for $\vec{B} \parallel [101]$ in Cu. It involves electrons lying on planes passing through the necks, as shown in Fig. 1. It has previously been observed with compressional waves.[2,3] We reported[3] a surprisingly large and rapid splitting of the fundamental resonance peak as $\vec{B}$ is rotated away from [101].

Figure 1 also shows the open orbit which runs along [111] for $\vec{B} \parallel [121]$. This is sometimes called the primary open orbit in Cu. It was the only one observed in the earlier magnetoacoustic experiments[4] using smaller values of ql. ($\vec{q}$ is the sound propagation vector and l is the electron mean free path.)

In this paper we compare the behavior of the resonances for the two open orbits as $\vec{B}$ is made parallel and perpendicular to $\vec{\epsilon}$. We call attention to the correlation between the orbit shapes and the amplitudes of the harmonics of the open-orbit resonances.

II. EXPERIMENTAL METHOD

The Cu specimen used in these experiments has a residual resistance ratio of about 35 000.[5] Its length in the direction of propagation is 1.25 cm. The specimen was mounted in a tiltable holder so that its axes could be precisely aligned in the magnetic field using the method described earlier.[6]

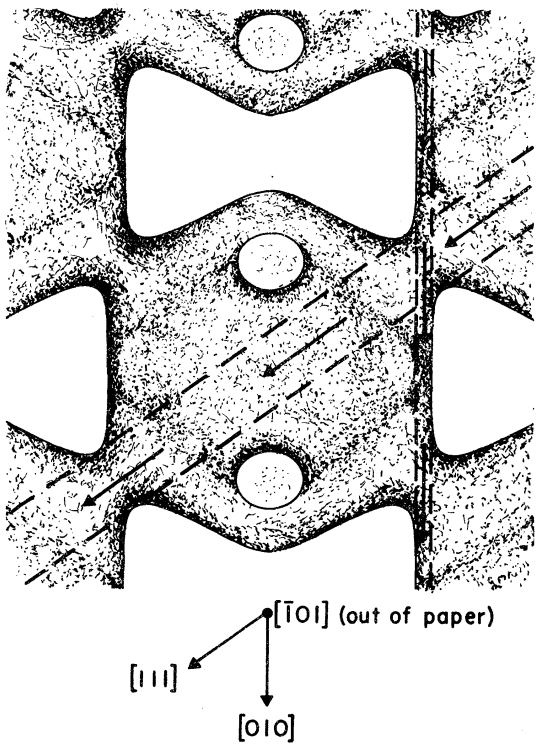

FIG. 1. Primary ([111] directed) and secondary ([010] directed) open orbits on the Cu Fermi surface (taken from Ref. 3).